INVESTIGATION OF DILUTE MAGNETIC SYSTEMS WITH SPIN-1 ISING MODEL IN THE FRAME OF GENERALIZED STATISTICAL MECHANICS

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Abstract

In this study the magnetization phenomenon has been investigated as a behavior of interacting elementary moments ensemble, with the help of Ising model [1] in the frame of non-extensive statistical mechanics. To investigate the physical systems with three states and two order parameters, the spin-1 single lattice Ising model or three states systems are used. In the manner of this model thermodynamical properties of a great deal of physical phenomena such as ferromagnetism in bilateral alloys, liquid mixtures, liquid-crystal mixtures, freezing, magnetic orderliness, phase transformations, semi-stable and unstable states, ordered and disordered transitions [2,3,4,5].

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1 Introduction

In this study, taking spin-1 Ising systems as the model dilute magnetic systems have been investigated in the frame of non-extensive statistics [6,7,8,9]. The general Hamiltonian of next nearest pair interaction spin-1 Ising systems is in the form

$$\begin{aligned} H = -J \sum_{<ij>} S_i S_j - K \sum_{<ij>} S_i^2 S_j^2 - \\ D \sum_{j=1}^{N} S_j^2 - H \sum_{j=1}^{N} - L \sum_{<ij>} S_i Q_j - \\ M \sum_{<ij>} S_i S^j (S_i + S_j) \end{aligned} \tag{1}$$

where J, K, D, H, L, M and N are bilinear exchange interaction constant, biquadratic exchange interaction constant, crystal field interaction constant, magnetic field due to S', dipole-quadropole interaction constant, magnetic perturbation of third degree and number of lattice points respectively. It the systems stay in semi-stable state or phase their properties change considerably. For examples, some alloys or metals lead to amorphons (glassy metal) structure when they are rapidly cooled down. This structure namely the phase is a semi-stable state. In this manner, some of the characteristics of the alloys or metals such as magnetic properties, resistance against corrosion, exhausting, wearing and hardness improve considerably. This Hamiltonian includes all possible terms when $s_i^\beta = s_i$ it does not include higher order powers of spin.

2 Dilute Systems

Dilute magnetic system is a system which is obtained by inclusion of non-magnetic atoms to magnetic atoms. Exhibition of magnetic property of such systems is possible when the concentration of the magnetic atoms reaches to a certain value. Dilute magnetism is given by the expression $A_p B_{1-p} C$ where A shows magnetic, B non-magnetic and C purely magnetic states. The Hamiltonian of such a system is defined in the form

$$H = -\sum_{<ij>} S_i S_j J n_i n_j \tag{2}$$

which is obtained by taking M=K=L=0 in Eq.(1). In this equation S_i and s_j are the spin vectors of i th and j th atoms, n_i and n_j are spin disorder variables taking the values 0 and 1 whose average value gives the magnetic concentration c. J is exchange energy.

Table 1: Spin Shaping Probabilities.

Shaping of Pairs	Probability	Energy	μ_i	Spin	Probability
1-1	y_{11}	$-(\frac{J}{2}) + \epsilon_{11}$	1	1	x_1
1-2	y_{12}	ϵ_{12}	1	2	x_2
1-3	y_{13}	$+(\frac{J}{2}) + \epsilon_{13}$	1	3	x_3
2-1	y_{21}	ϵ_{21}	1		
2-2	y_{22}	ϵ_{22}	1		
2-3	y_{23}	ϵ_{23}	1		
3-1	y_{31}	$+(\frac{J}{2}) + \epsilon_{31}$	1		
3-2	y_{32}	ϵ_{32}	1		
3-3	y_{33}	$-(\frac{J}{2}) + \epsilon_{33}$	1		

In table 1 where the spin shaping probabilities are presented, ν_i are different shping numbers having same probability. ϵ_{11}, ϵ_{12}, ϵ_{13}, ϵ_{21}, ϵ_{22}, ϵ_{23}, ϵ_{31}, ϵ_{32} and ϵ_{33} are atomic interactions. If magnetic atoms are grouped as A and B denotes the atoms which are not magnetic then $\epsilon_{11} = \epsilon_{13} = \epsilon_{33} = \epsilon_{AA}, \epsilon_{12} = \epsilon_{32} = \epsilon_{21} = \epsilon_{23} = \epsilon_{AB} and \epsilon_{22} = \epsilon_{BB}$. The spin directions of the magnetic atoms are 1 and 3 and the directions of the atoms which are not magnetic is 2. The probabilities of the atoms having spins in the upward directions is x_1, ,n downward is x_3 and the atoms that are not magnetic is x_2. Since the probabilities having symmetry are equal as a result $y_{12} = y_{21}, y_{23} = y_{32}$ and $y_{13} = y_{31}$. The shaping of pairs at the lattice point takes place in nine different form and these shaping have been given in Table 1.

3 Free Energy of the System

The energy per atom of such a system is

$$\frac{E}{N} = J\gamma(y_{13} - \frac{y_{11}+y_{33}}{2}) + \frac{\gamma}{2}[\epsilon_{AA}(y_{11}+2y_{13}+y_{33}) + 2\epsilon_{AB} + (y_{12}+y_{23}) + \epsilon_{BB}y_{22}] + (y_{11}+y_{12}-y_{33}-y_{32})\beta H \quad (3)$$

where γ is the number of nearest lattice points, N is the number of lattice points of the system, H is the external magnetic field and $\beta = \frac{1}{k_B T}$. Using the weight factor x_i as the internal variable which has been developed for three state systems and y_{ij} as double variable, the statistical weight of the spin-1 Ising system could be written as;

$$[W]^{\frac{1}{N}} = \frac{[\prod_{i=1}^{3}(x_i L)!]^{\gamma-1}}{L!^{\frac{\gamma}{2}-1}[\prod_{i,j=1}^{3}(y_{ij}L)!]^{\frac{\gamma}{2}}} \quad (4)$$

where N is the number of lattice points in the system and 1 is the number of systems in the ensemble. On the other hand the definition of entropy is

$$S = \frac{k_B}{lnW}. \quad (5)$$

When the entropy is calculated for a single system (L=1)

$$\frac{S}{N} = k_B[(\gamma-1)\sum_{i=1}^{3} x_i ln x_i - (\frac{\gamma}{2})\sum_{i,j=1}^{3} y_{ij} ln y_{ij}] \quad (6)$$

is found. Thus free energy becomes:

$$F = E - TS.$$

Using the expressions in Table 1, free energy takes the form

$$F = J\gamma(y_{13} - \frac{y_{11}+y_{33}}{2}) + \frac{\gamma}{2}[\epsilon_{AA}(y_{11}+2y_{13}+y_{33}) + 2\epsilon_{AB}(y_{12}+y_{23}) + \epsilon_{BB}y_{22}] - (y_{11}+y_{12}-y_{33}-y_{32})\beta H - \frac{1}{\beta}[(\gamma-1)\sum_{i=1}^{3} x_i ln x_i - (\frac{\gamma}{2})\sum_{i,j=1}^{3} y_{ij} ln y_{ij}] \quad (7)$$

4 Obtaining the Equilibrium State of the Dilute System

The equilibrium state of a dilute system could be obtained by the calculus of variations. For this purpose three independent variables η, ξ_1 and ξ_2 are defined:

$$\eta = \frac{y_{13} + y_{31}}{2} = y_{13} \tag{8}$$

$$2\xi_1 = x_1 - x_2 \tag{9}$$

$$2\xi_2 = y_{12} - y_{32} \tag{10}$$

where η indicates the energy variation, ξ_1 represents magnetization and ξ_2 shows the abundance of the upward spins with respect to the downward spins of A atoms which are neighbors of B atoms.

5 Equilibrium State of the Dilute System in the Frame of Non-extensive Statistical Mechanics

Until 1998 all of the physical quantities of statistical systems were obtained by Boltzmann-Gibbs statistics. According to Boltzmann-Gibbs statistics, macro quantities such as free energy, entropy and internal energy of a statistical system were accepted as extensive quantities. In 1998 a generalization in the Thermodynamical meaning has been carried aut to understand the structure or to solve a great number of unfamiliar systems and the generalization was inspired from the probability definition of the multifractal geometry. Magnetization is a process with a long range and memory. Such systems are non-extensive. Thus magnetization will be investigated in the frame of non-extensive statistical mechanics. This generalization is the parametrization of all of the statistical quantities by a parameter q. In the limit $q \to 1$ the statistics under investigation reduces to Boltzmann-Gibbs statistics. For the values of q different than 1, macro quantities such as internal energy, free energy and entropy in Boltzmann-Gibbs statistics are not extensive quantities in other words they are non-extensive. For generalization, mathematical expressions obtained from non-extensive statistical mechanics are introduced;

$$\ln_q x = \frac{x^{1-q}-1}{1-q} and$$
$$\exp_q^x = \{[1+(1-q)x]^{\frac{1}{1-q}} if 1+(1-q)x \geq 0$$
$$0 else. \tag{11}$$

On the other hand, when Eq.(11a) is written down for any function $f(x)$, its derivative becomes

$$[ln_q f(x) = \frac{f(x)^{1-q}-1}{1-q}]^l = \frac{(1-q)f(x)^- q f^l(x)}{1-q} = \frac{f^l(x)}{f(x)^q} \tag{12}$$

In this system, the equilibrium state is determined using the variation of the free energy with respect to parameters η, ξ_1 and ξ_2 given above. The variation of free energy leads to nonlinear equations:

$$y_{11}y_{33} = y_{13}^2 e_q^{\frac{2J}{kT}} \tag{13}$$

$$(\frac{y_{11}}{y_{33}})^{\frac{\gamma}{2}} = (\frac{x_1}{x_3})^{\gamma-1} e_q^{\frac{2\beta H}{k_B T}} e_q^{(\gamma-1)(x_3^{1-q}-x_1^{1-q})} \tag{14}$$

$$\frac{y_{11}}{y_{33}} = (\frac{y_{12}}{y_{32}})^2 e_q^{2(y_{12}^{1-q}-y_{32}^{1-q})+(y_{33}^{1-q}-y_{11}^{1-q})} \tag{15}$$

Starting from Table 1 and taking $x_3^{1-q} \cong x_1^{1-q}$ in Eq.(13) and $y_{12}^{1-q} \cong y_{32}^{1-q}$ and $y_{33}^{1-q} \cong y_{11}^{1-q}$ in Eq.(14) these equations are
brought to simpler form:

$$y_{11}y_{33} = y_{13}^2 e_q^{\frac{2J}{k_B T}} \tag{16}$$

$$(\frac{y_{11}}{y_{33}})^{\frac{\gamma}{2}} = (\frac{x_1}{x_3})^{\gamma-1} e_q^{\frac{2\beta H}{k_B T}} \tag{17}$$

$$\frac{y_{11}}{y_{33}} = [\frac{y_{12}}{y_{32}}]^2. \tag{18}$$

It is obvious that the solutions of these equations could be obtained depending on the entropy parameter q. In order to proceed to physically measurable results, let us relate the probabilities with the relevant concentrations. Existence probability of the magnetic atoms in the lattice point is n_A and the probability for the atoms that are not magnetic is n_B. Therefore

$$n_A = x_1 + x_3 or n_A = y_{11} + y_{12} + y_{13} + y_{31} + y_{32} + y_{33} \tag{19}$$

$$n_B = x_2 or n_B = y_{21} + y_{22} + y_{32} \tag{20}$$

$$n_{AA} = y_{11} + y_{13} + y_{31} + y_{33} \tag{21}$$

$$n_{AB} = y_{12} + y_{13} + y_{32} \tag{22}$$

$$n_{BA} = y_{21} + y_{23} \tag{23}$$

$$n_{BB} = y_{22}. \tag{24}$$

Writing $c = \eta_A$ in other wards by taking the concentration of the magnetic atoms above equations could be expressed in terms of c:

$$n_{AA} = c^2 \tag{25}$$

$$n_{AB} = c(1-c) \tag{26}$$

$$n_{BA} = c(1-c) \tag{27}$$

$$n_{BB} = (1-c)^2. \tag{28}$$

6 Calculation of the Orientation Probabilities

In order to solve the equations given above a transformation given by

$$\frac{x_1}{x_3} = e_q^{2\gamma t} \tag{29}$$

is used in Eqs.(15),(16) and (17) which leads to the solutions of these nonlinear equations:

$$\xi_1 = \frac{n_A}{2} \tanh_q(\gamma - 1)t. \tag{30}$$

The third parameter

$$\xi_2 = \frac{n_B}{2} \tanh_q(\gamma - 1)t \tag{31}$$

is obtained. Using these results the probabilities x_i and y_{ij} are found:

$$y_{11} = \frac{n_{AA} \exp_q^{2(\gamma-1)t}}{2[\cosh_q 2(\gamma - 1)t + e_q^{\frac{-J}{k_B T}}]} \tag{32}$$

$$y_{12} = y_{21} = \frac{n_{AB}}{2}(\tanh_q(\gamma - 1)t + 1) \tag{33}$$

$$y_{13} = y_{31} = \frac{n_{AA}}{2[\exp_q^{\frac{J}{k_B T}} \cosh_q 2(\gamma - 1)t + 1]} \tag{34}$$

$$y_{22} = n_{BB} \tag{35}$$

$$y_{23} = y_{32} = \frac{n_{AB}}{2}(1 - \tanh_q(\gamma - 1)t) \tag{36}$$

$$y_{33} = \frac{n_{AA}}{2 \exp_q^{\frac{J}{k_B T}} [\cosh_q 2(\gamma - 1}) t + \exp_q^{\frac{-J}{k_B T}}] . \tag{37}$$

On the other hand the internal variables x_i are determined as,

$$x_1 = \frac{n_A(1 + \tanh_q \gamma t)}{2} \tag{38}$$

$$x_2 = n_A \tag{39}$$

$$x_3 = \frac{n_A(1 - \tanh_q \gamma t)}{2} \tag{40}$$

7 Determination of the Physical Quantities

When the relation between the parameter t and temperature is determined by using the obtained probabilities, the nonlinear equations and expression related to the concentration one gets:

$$e_q^{\frac{J}{kT}} = \frac{n_A \tanh_q \gamma t}{\cosh_q 2(\gamma - 1)t[n_{AA} \tanh_q 2(\gamma - 1)t + n_{AB} \tanh_q(\gamma - 1)t - n_A \tanh_q \gamma t]} - \frac{n_{AB} \tanh_q(\gamma - 1)t}{\cosh_q 2(\gamma - 1)t[n_{AA} \tanh_q 2(\gamma - 1)t + n_{AB} \tanh_q(\gamma - 1)t - n_A \tanh_q \gamma t]} \tag{41}$$

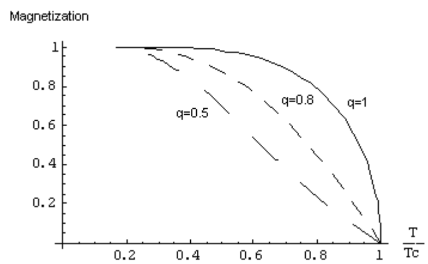

Figure 1: Variation of magnetization with respect to temperature for simple cubic structure ($\gamma = 6.$) at a certain concentration (c=1) and for different g values (Eq(29)). $\tau = f(T)$ plot.

According to Eq.(29) the magnetization is

$$\tau_q = 2\xi_1 or \tau_q = n_A \tanh(q\gamma t) \tag{42}$$

Variation of the magnetization with respect to temperature at a certain concentration value (c=1) for different q values, in other words the plot of the function $\tau_q = f(T)$ is given in Fig.(1). In the figure solid line refers to $q \cong 1$, closer spaced dashed line shows the plot for q=0.8 and wider spaced dashed line for $q = 0.5$.

The susceptibility is expressed as

$$\frac{1}{\chi_q} = \frac{kT[1 + e_q^{\frac{J}{kT}} \cosh_q 2(\gamma - 1)t](n_A - \gamma n_{AA} - n_{AA}) + 2n_{AA}(\gamma - 1)}{\beta^2[1 + e_q^{\frac{J}{kT}} \cosh_q 2(\gamma - 1)t](n_A^2 + n_{AA}n_A) - n_A n_{AA}} \tag{43}$$

In Fig.(2) the variation of susceptibility with respect to temperature at a certain concentration value (c=1) for different q values, in other words the plot of the function $\chi_q = f(T)$ is represented. In this plot solid line correspond to $q \cong 1$ and the dashed line to $q = 0.5$.

When the magnetic part of the energy is taken under consideration one writes:

$$\frac{E_q}{N} = \frac{\gamma J}{4}(4\eta - n_{AA}) \tag{44}$$

$$\frac{E_q}{N} = \frac{-\gamma J}{4} n_{AA} [\frac{1 - e^{\frac{-J}{kT}} \sec(h_q) 2(\gamma - 1)t}{1 + e^{\frac{-J}{kT}} \sec(h_q) 2(\gamma - 1)t}] \tag{45}$$

Using these expressions the specific heat is found to be;

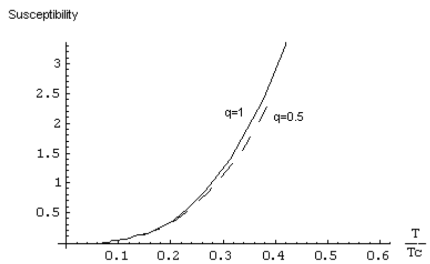

Figure 2: Variation of susceptibility heat with respect to temperature for simple cubic structure ($\gamma = 6$).) at a certain concentration ($c = 1$) and for different g values (Eq(42)). $\chi = f(T)$ plot.

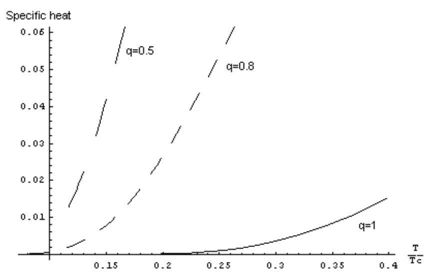

Figure 3: Variation of specific heat with respect to temperature for simple cubic structure ($\gamma = 6.$) at a certain concentration (c=1) and for different g values (Eq(44)). $SI = f(T)$ plot.

$$\frac{C_q}{k_B N} = \frac{1}{k_B N}\frac{dE_q}{dT}). \tag{46}$$

$$\frac{C_q}{kN} = \frac{\gamma J}{4k} n_{AA} \frac{d}{dT}[\frac{e^{\frac{-J}{kT}}\sec(h_q)2(\gamma-1)t-1}{e^{\frac{-J}{kT}}\sec(h_q)2(\gamma-1)t+1}] \tag{47}$$

In Fig.(3) the variation of the specific heat with respect to temperature at a certain value of concentration (c=1) for different g values, in other words $c_q = f(T)$ plot is shown; where the solid line is for $q \cong 1$, closer spaced dashed line for $q \cong 0.8$ and wider spaced dashed line for $q = 0.5$.

8 Conclusions

In this study; by considering the dilute magnetic systems as an ensemble of interacting elementary moments and in this context with the help of

spin-1 Ising model; they are investigated microscopic level. Due to the statistical mechanics a bridge has been constructed between microscopic level approach and macroscopic experimental results. Magnetization is a long range phenomenon with a memory. Such systems are non-extensive. For this reason; magnetization has been considered in the frame of non-extensive statistical mechanics. Starting with the standard approach the generalization process proceeds. Same of the experimental studies where this type of systems are investigated has also been given [10,11,12]. In this study the variations of magnetization, susceptibility and specific heat with respect to temperature have been investigated. It is observed that; at different values of the entropic index q, in other words when q is decreasing, magnetization exhibits a linear variation rather than a parabolic one. On the other hand, it seen that the susceptibility does not undergo any change with q values. In the specific heat however, with decreasing q temperature dependence increases.

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